Supplementary Information file

Novel low energy hydrogen-deuterium isotope breakthrough separation using a trapdoor zeolite

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1.1 Supplementary figures

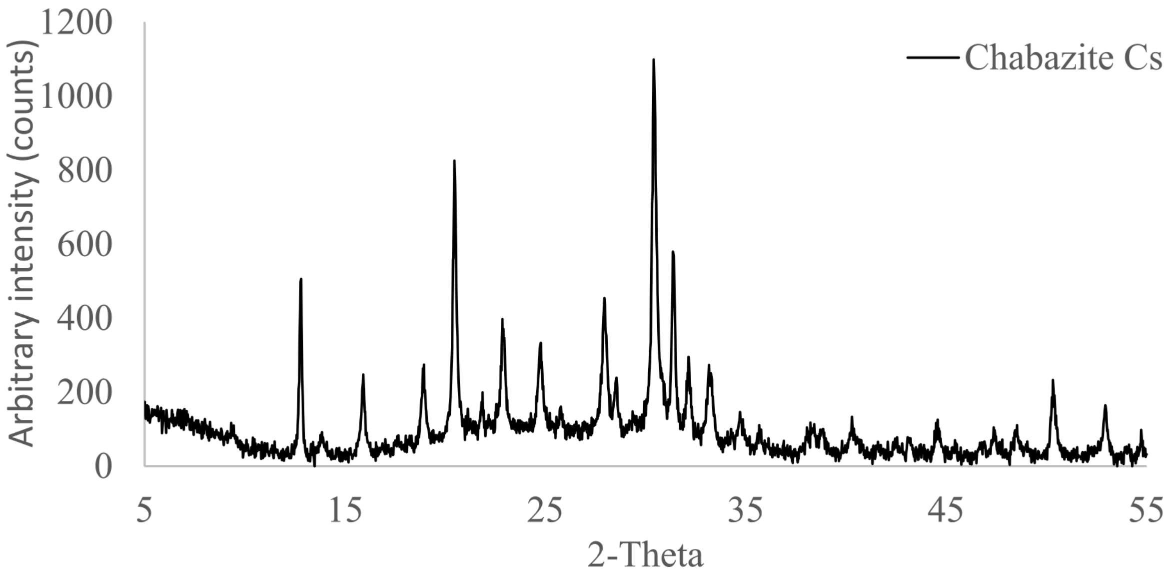

Figure S1: Powder X-Ray Diffraction (PXRD) pattern of the as received Cs-chabazite from the Webley lab (University of Melbourne, Australia). A 2-theta range of 5-55 with a Cu-$K\alpha1$ radiation source of λ = 0.1541 nm was used, and 40 kV and 40 mA power rating.

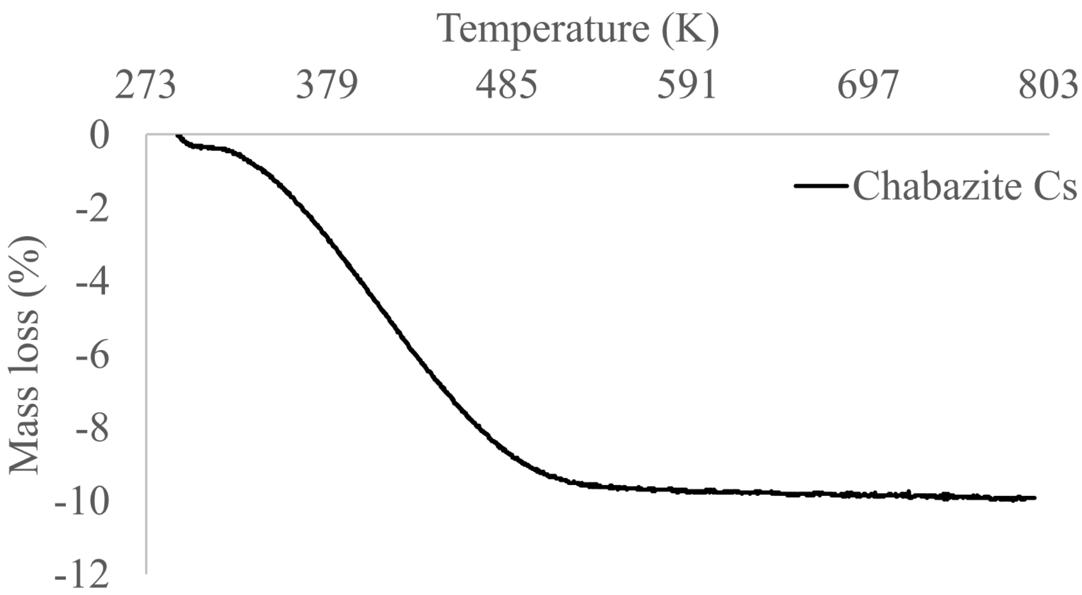

Figure S2: Thermogravimetric Analysis (TGA) on Cs-chabazite in a nitrogen atmosphere, from 273-823 K, with a scan rate of 5 $K.min^{-1}$. ~10 wt% mass loss due to moisture desorption on a 26 mg sample.

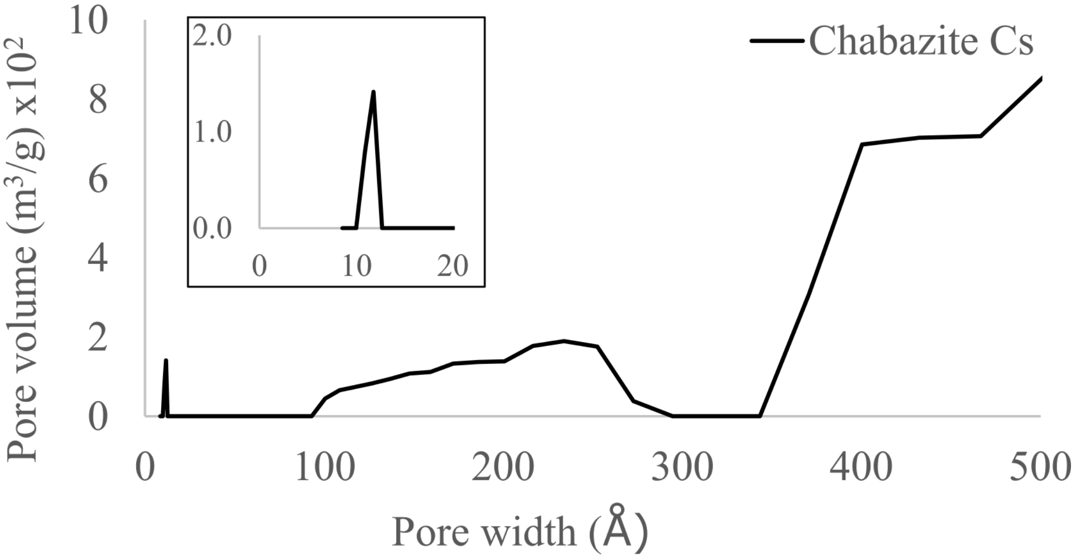

Figure S3: Density Functional Theory Pore Size Distribution (DFT-PSD) analysis of nitrogen sorption isotherms on Cs-CHA at 77 K, represented as incremental pore volume vs pore width. Insert shows the microporosity at ~11 Å (internal supercavities reported as 6.7 x 6.7 Å).

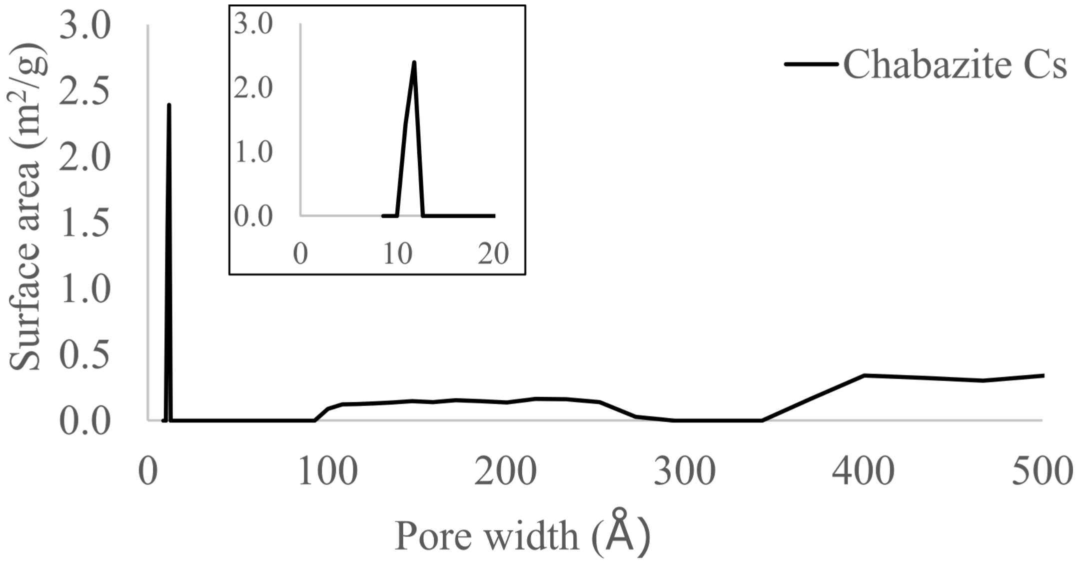

Figure S4: Density Functional Theory Pore Size Distribution (DFT-PSD), analysis of nitrogen sorption isotherms on Cs-CHA at 77 K, represented as incremental surface area vs pore width. Insert shows the microporosity at ~11 Å.

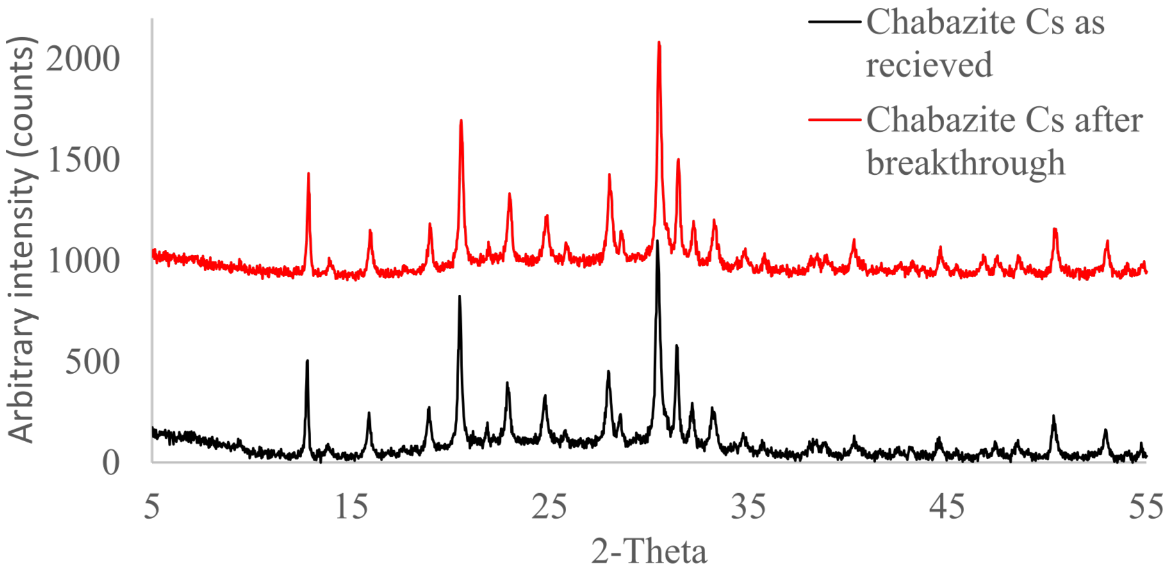

Figure S5: Powder X-Ray Diffraction (PXRD) pattern of the as received Cs-chabazite from the Webley lab (University of Melbourne, Australia), compared to the same sample post-breakthrough. Phase purity was unaffected by breakthrough cycling and heating (>20 heating cycles) within the reactor. A 2-theta range of 5-55 with a Cu-$K\alpha1$ radiation source of λ = 0.1541 nm was used, and 40 kV and 40 mA power rating.

1.2 Supplementary information

To determine the goodness of fit, the chi-squared method was used. The χ^2 value was first calculated by summing the results of the squared observed values minus the expected values, all over the expected values for C/C_0 (Eq. S1). The χ^2 values were then compared with a χ^2 *vs.* degrees of freedom chart to obtain the p-value, which is the probability of the results being due to chance.

$$\chi^2 = \sum_{i=1}^{n} \frac{(O_i - E_i)^2}{E_i}$$

Eq. S1

To calculate the bulk density (ρ_B) within the reactor, the sample mass (m) was divided by the bed volume (V_B) displaced by the sample. The bed volume displaced was calculated by multiplying the reactor inside cross sectional area (πr^2) by the length (H) of the packed bed (Eq. S2), which was measured using compression pins within the reactor.

$$\rho_B = \frac{m}{(\pi r^2)\, H}$$

Eq. S2

The voidage, or interstitial space (ϵ), was calculated using Eq. S3,

$$\in = \frac{1 - m}{\rho_p A H}$$

Eq. S3

where m is the mass of the sample, ρ_P is the density of the sample, A is the cross sectional area and H is the bed length.